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Measurements of a component of the piezo-optic tensor of Si by reflectance difference spectroscopy

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The component $\tilde{P}_{44}(\omega)$ of the piezo-optic tensor of Si was measured by reflectance difference spectroscopy (RDS). Taking advantage of the high sensitivity of RDS, the measurements were carried out under a much lower stress field compared to the previous report using ellipsometry. The spectra measured at 2.1 MPa by RDS agree well with literature data obtained at 2 GPa by ellipsometry. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1586965]

I. INTRODUCTION

The electric and optical properties of semiconductors are modified by strain which is caused by externally applied stress or lattice mismatch. For example, strained Si epitaxial layers have been attracting significant interest because of their high electron mobility.[1] The modification of optical properties by strain is caused by the changes in the electronic structure.[2] Strain modified optical responses of the materials are represented by the piezo-optic tensor, $\tilde{P}_{ijkl}(\omega)$. It is a fundamental quantity not only for optical device application but also for measurements of strain by optical methods.

The components of $\tilde{P}_{ijkl}(\omega)$ were determined using spectroscopic ellipsometry for Ge,[3] GaAs,[4] Si,[5] and InP.[6] Recently for ZnSe and ZnTe[7] it was reported that piezo-optic coefficients can also be determined by reflectance difference spectroscopy (RDS). RDS measures the difference of the normal-incidence reflectances between two orthogonal linear polarization directions.[8] Using RDS, these coefficients can be obtained under much lower stress fields of a few megapascal compared with the case of the ellipsometry measurements where stress as high as a few gigapascal is required. Measurements under lower fields have several advantages. First of all, the measurements can be performed on brittle materials or thin film samples which cannot withstand large stresses. Another important advantage is that the results are free from errors caused by stress-induced surface deformation.

Within a linear response regime, the stress-induced change in a complex dielectric tensor $\Delta\tilde{\epsilon}_{ij}$ is proportional to an externally applied stress F_{kl}:

$$\Delta\tilde{\epsilon}_{ij}=\tilde{P}_{ijkl}F_{kl}, \tag{1}$$

where $\tilde{P}_{ijkl}$ is a piezo-optic tensor and the suffixes i, j, k, and l represent one of the rectangular coordinate axes 1, 2, and 3. Another definition

$$\Delta\tilde{\epsilon}_{ij}=-\tilde{\epsilon}^2\tilde{Q}_{ijkl}F_{kl} \tag{2}$$

by Nye[9] is also frequently used. In this article we choose the definition Eq. (1) as Etchegoin and co-workers did[5] to compare with their data.

In diamond type (point group $d3m$) crystals, there are three independent components of the piezo-optic tensor: $\tilde{P}_{11}$, $\tilde{P}_{12}$, and $\tilde{P}_{44}$. The irreducible components are $\tilde{P}_{44}$ (stress of $\Gamma_{25'}$ symmetry, i.e., shear stress), $\tilde{P}_{11}-\tilde{P}_{12}$ (stress of Γ_{12} symmetry, i.e., axial stress) and $\tilde{P}_{11}+2\tilde{P}_{12}$ (stress of Γ_1 symmetry, i.e., hydrostatic stress). RDS cannot measure $\tilde{P}_{11}+2\tilde{P}_{12}$ because the isotropic stress causes no anisotropy that RDS measures.

II. RELATION BETWEEN RD SIGNAL AND PIEZO-OPTIC TENSOR

The RD signal for any two orthogonal directions of polarization(A axis and B axis) is defined as

$$\frac{\Delta\tilde{r}}{\tilde{r}}=\frac{2(\tilde{r}_A-\tilde{r}_B)}{(\tilde{r}_A+\tilde{r}_B)}. \tag{3}$$

The measurement results are generally displayed in terms of $\Delta\tilde{r}/\tilde{r}=\Delta r/r+i\cdot\Delta\theta$, where $\tilde{r}=r\cdot\exp(i\theta)$ is complex reflectance. We can experimentally obtain both reliable $\Delta r/r$ and $\Delta\theta$ data. $\Delta\tilde{r}/\tilde{r}$ is coverted to the dielectric anisotropy $\Delta\tilde{\epsilon}_1$ adopting a three phase model which takes into account the contribution of the thin oxide layer on Si. The normal-incidence reflectance $\tilde{r}$ in the three phase model is given as

$$\tilde{r}=\frac{\tilde{r}_2+\tilde{r}_1\exp(i2\tilde{\delta}_2)}{1+\tilde{r}_1\tilde{r}_2\exp(i2\tilde{\delta}_2)}, \tag{4a}$$

$$\tilde{r}_1=(\tilde{n}_1-\tilde{n}_2)/(\tilde{n}_1+\tilde{n}_2), \tag{4b}$$

and

$$\tilde{r}_2=(1-\tilde{n}_2)/(1+\tilde{n}_2), \tag{4c}$$

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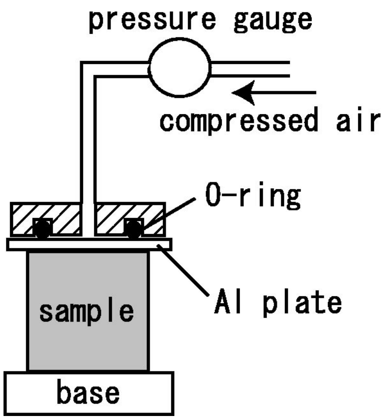

FIG. 1. Schematic illustration of the measurement system.

where $\tilde{\delta}_2 = 2\pi\tilde{n}_2 d_2/\lambda$, $\tilde{n}_1$ and $\tilde{n}_2$ are the complex refractive indices of the Si and the silicon oxide overlayer, respectively, d_2 is the thickness of the silicon oxide layer, and λ is the wavelength of the incident light. $\tilde{r}_1$ and $\tilde{r}_2$ are the complex reflectances between the silicon oxide overlayer and the bulk Si, and between the ambient and the silicon oxide overlayer, respectively. The relation between $\Delta\tilde{\epsilon}_1$ and $\Delta\tilde{r}/\tilde{r}$ is given by introducing the partial derivative of $\tilde{r}$ with respect to $\tilde{n}_1$:

$$\frac{\Delta\tilde{r}}{\tilde{r}} = \frac{1}{\tilde{r}}\frac{\partial\tilde{r}}{\partial\tilde{n}_1}\cdot\Delta\tilde{n}_1 = \frac{1}{2\tilde{n}_1\tilde{r}}\frac{\partial\tilde{r}}{\partial\tilde{n}_1}\cdot\Delta\tilde{\epsilon}_1. \tag{5}$$

In the case of anisotropy between $[1\bar{1}0]$ and $[110]$ polarizations in a (001) face due to the uniaxial stress F along $[1\bar{1}0]$, the stress-induced dielectric anisotropy $\Delta\tilde{\epsilon}_1$ is given by

$$\Delta\tilde{\epsilon}_1 = (\tilde{P}_{11}+\tilde{P}_{12}+\tilde{P}_{44})F - (\tilde{P}_{11}+\tilde{P}_{12}-\tilde{P}_{44})F = 2\tilde{P}_{44}F. \tag{6}$$

In the case of anisotropy between $[110]$ and $[001]$ in the $(1\bar{1}0)$ face due to the uniaxial stress F along $[001]$, $\Delta\tilde{\epsilon}_1$ is given by

$$\Delta\tilde{\epsilon}_1 = (\tilde{P}_{11}+\tilde{P}_{12})F - 2\tilde{P}_{12}F = (\tilde{P}_{11}-\tilde{P}_{12})F. \tag{7}$$

By substituting Eq. (6) or Eq. (7) into Eq. (5), we can respectively obtain $\tilde{P}_{44}$ and $\tilde{P}_{11}-\tilde{P}_{12}$ from RD spectra. In the case of Eq. (6), the relation between RD spectra and the piezo-optic tensor component $\tilde{P}_{44}$ is described by

$$\tilde{P}_{44} = \frac{\tilde{n}_1\tilde{r}}{F}\frac{\partial\tilde{n}_1}{\partial\tilde{r}}\frac{\Delta\tilde{r}}{\tilde{r}}. \tag{8}$$

On the right-hand side of this equation, $\Delta\tilde{r}/\tilde{r}$ is obtained by measureing the difference between RD spectra with and without stress. We called it the differential RD (DRD) spectra in this article.

III. EXPERIMENT

The experiment was done using a sample of undoped Si cut into a cubic shape of 10×10×10 mm. The reflection plane was (001) with a uniaxial stress of 2.1 MPa along [110] applied by compressed air. A schematic picture of the measurement system is shown in Fig. 1. Applied stress was directly measured by an air pressure gauge and corrected for the effective gas-contact area. To ensure uniform application of stress, we inserted an Al plate between the sample and the O ring.

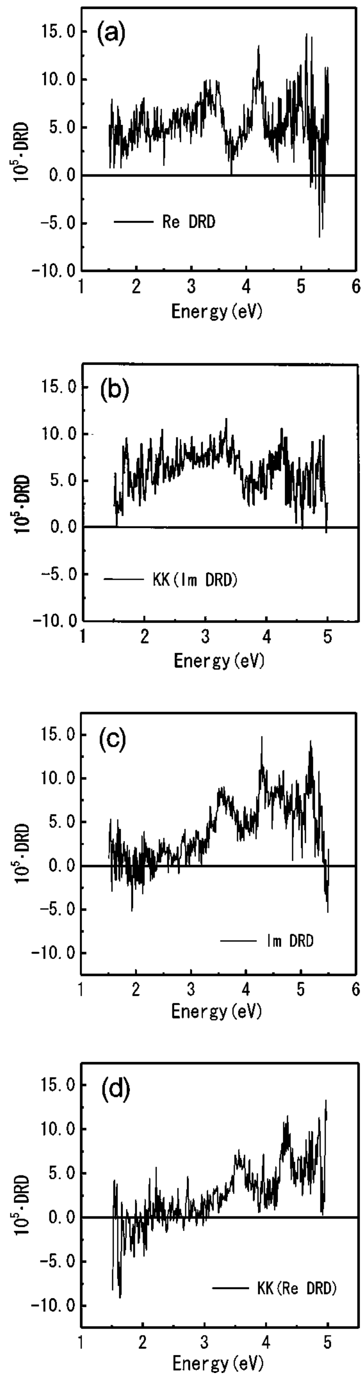

FIG. 2. DRD spectra of Si from 1.5 to 5.5 eV: (a) real part; (b) KK conjugate of imaginary part; (c) imaginary part; and (d) KK conjugate of real part.

F in Eq. (8) was measured by a pressure gauge as described above. $\partial\tilde{r}/\partial\tilde{n}_1$ and $\tilde{r}$ can be calculated using the dielectric functions without stress. $\tilde{n}_1$, $\tilde{n}_2$ and the overlayer thickness $d_2 = 20$ Å were measured by spectroscopic ellipsometry. The dielectric function of Si measured by Aspnes it *et al.*[10] and that of silicon oxide by Borgogno *et al.*[11] were used.

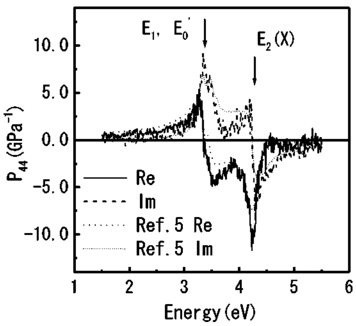

FIG. 3. The $\widetilde{P}_{44}$ spectra of Si. The reference data were taken from Ref. 5.

In the present work, we only measured the irreducible piezo-optic tensor components $\widetilde{P}_{44}$ of Si, using RDS. This is because a sample was not available to measure the $\widetilde{P}_{11} - \widetilde{P}_{12}$ component. The results are compared to the previous report by Etchegoin *et al.*[5] using ellipsometry under 2.0 GPa.

Since the DRD amplitude was small, it is critically important to have a stable base line of the RD spectra. The measurement system was carefully tuned to minimize the base line drift.

IV. RESULTS AND DISCUSSION

The real and imaginary parts of the obtained DRD spectra and the Kramers–Kronig (KK) conjugates of their counterparts are shown in Fig. 2. The agreement between the measured spectra and their KK conjugates is good. This agreement verifies that the spectra were measured correctly. Figure 3 shows the $\widetilde{P}_{44}$ spectra obtained by converting the data of Fig. 2 using Eq. (8). The line shape almost reproduces the result reported in Ref. 5. The peak splitting at the E_1 transition energy near 3.5 eV[5] is also observed by RDS. The largest difference between ellipsometry and RDS is observed in the energy range from 3.5 to 4 eV. The origin of this difference is still unknown. We note, however, that our $\widetilde{P}_{44}$ spectra are essencially reproduced by five independent mesurements.

Here we point out two advantages of the present method in eliminating the possible sources of errors. First, since the applied stress is small, the Si surface can be regarded as an ideally flat reflection plane. Second, RDS directly measures the irreducible components of the piezo-optic tensor. To obtain the same components from the ellipsometry measurements, one has to measure two spectra at different azimuth angles and take the difference between them.

V. SUMMARY

We measured the piezo-optic coefficient $\widetilde{P}_{44}$ of Si by RDS at stresses as low as 2.1 MPa. The feasures around E_1 and $E_1+\Delta_1$ were in good agreement with literature data obtained at 2.0 GPa using ellipsometry.

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